Uncertainties Assessment in Nuclear Data Evaluations

P.Talou, P.G.Young and M.B.Chadwick
T-16, Nuclear Physics Group, LANL

Role & Importance of accurate nuclear data evaluations

Evaluations work in T-16

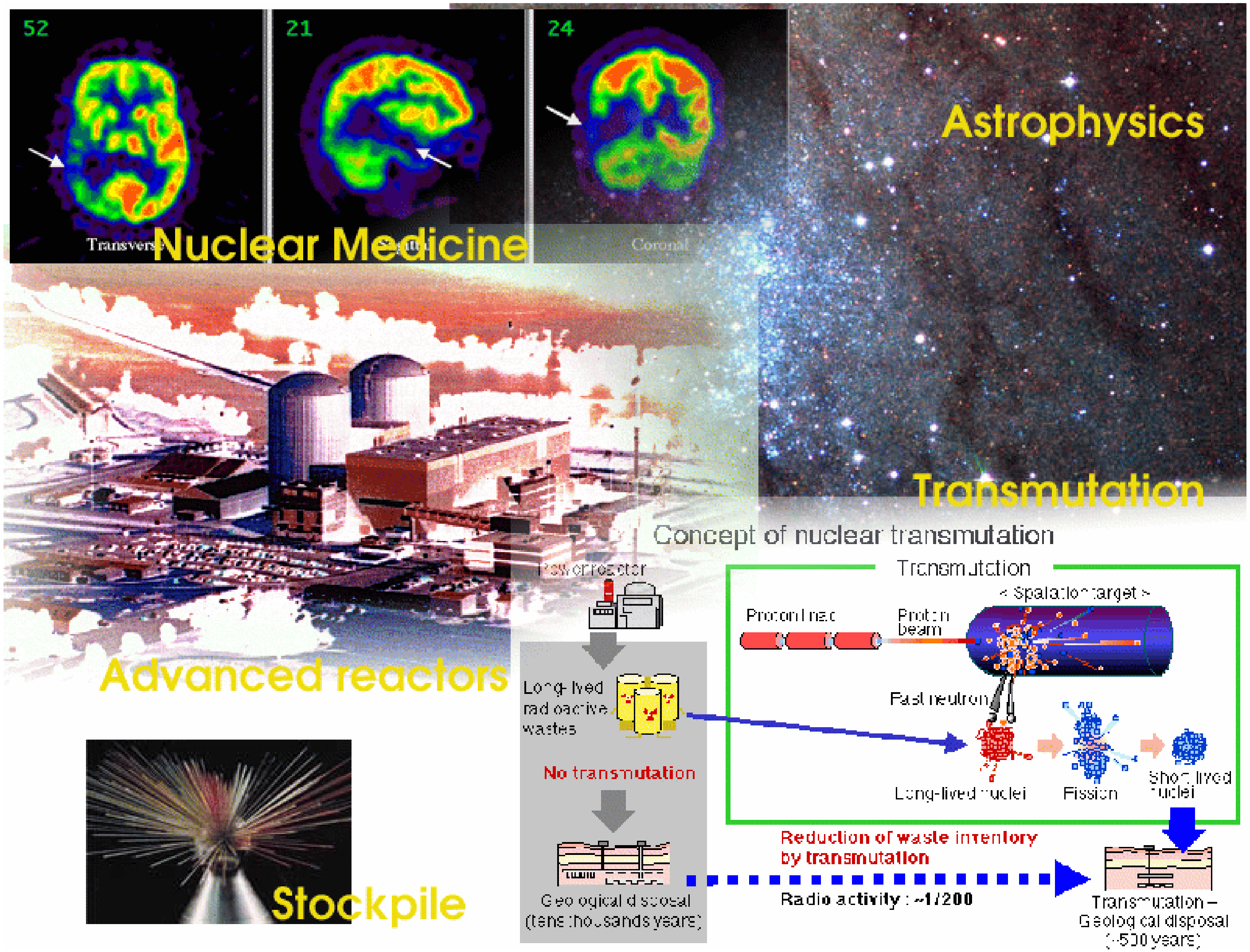
Statistical Analysis & Bayesian Inference Scheme.

^{239}Pu(n,f) & ^{235}U(n,f) cross-sections evaluations:
The importance of raw data analysis and "clean-up"

Improvements?

Role & Importance of Nuclear Data Evaluations

Accurate nuclear reaction cross sections are crucial in many areas of nuclear physics & applications.



T-16 work on nuclear data evaluations

→ Nuclear reaction modeling: Hauser-Feshbach statistical theory of the compound nucleus, direct reactions, preequilibrium effects, intra-nuclear cascade, R-matrix analysis of reactions on light-elements,...

→ Many physics "ingredients" enter in such modeling: nuclear masses, fission barriers, nuclear level densities, ...

→ Creation of **ENDF files** (Evaluated Nuclear Data File): electronic files containing valuable informations on reaction cross-sections, energy-angle spectrum of emitted particles, recoil heavy nuclei, etc.

→ These evaluations are the result of a **combination of theoretical modeling and experimental data analysis**.

→ ***Bayesian inference scheme*** to get "best estimates" from experimental data (underlying goal: reducing the role of systematic errors in experimental setups).

A Practical Evaluation...

...usually involves **experimental data combined with theoretical modeling**. In some cases however, the evaluation has to rely on experimental data sets only (no available model reliable enough).

Statistical Analysis of Experimental Data Sets

- Mathematical tools: Bayesian inference scheme or/and simultaneous evaluation;
- Careful examination of experimental data sets;
  What is measured is rarely equivalent to what one seeks to obtain! The relationship between what is measured and what is sought must be specified in order to carry out a proper evaluation.

Good information on experimental conditions is crucial!

Statistical Data Evaluation (1)

1. Bayes' Theorem
2. Maximum likelihood condition
3. Generalized Least-Squares Method

D : a data set

Φ : a set of physical quantities (or parameters) to be determined

Bayes' theorem:

$$\boxed{P\ (\Phi \mid D) = L\ (D \mid \Phi) \times P_0(\Phi) \,/\, P\ (D)}$$

Posterior

Likelihood

Prior

- The prior gathers information available before acquiring the new data set D;
  The likelihood function gives the probability of observing D if the parameters Φ were indeed true.

- Iterative approach.

Statistical Data Evaluation (2)

Maximum likelihood condition

Likelihood:

$$\boxed{L(\mathbf{D},\mathbf{p}) \propto \exp\left\{(-\,1/2)\left[\mathbf{y}\text{-}\mathbf{f}(\mathbf{p})\right]^{+} V_{y}^{-1}\left[\mathbf{y}\text{-}\mathbf{f}(\mathbf{p})\right]\right\}}$$

Where $\mathbf{V_y}$ represents the experimental covariance matrix,
$\mathbf{p}$ is the parameters vector, and $\mathbf{f}(\mathbf{p})$ correspond to the experimental values $\{\mathbf{y}\}\equiv\mathbf{D}$.

Let us suppose that the prior includes an initial parameter set $\mathbf{p_0}$ (and corresponding covariance matrix $\mathbf{V_0}$), then the PME brings a multivariate normal distribution,

Prior:

$$P_0(\mathbf{p}) \propto \exp\left\{(-\,1/2)\left[\mathbf{p}\ \text{-}\mathbf{p_0}\right]^{+} \mathbf{V_0}^{-1}\left[\mathbf{p}\text{-}\mathbf{p_0}\right]\right\}$$

Statistical Data Evaluation (3)

The **Generalized Least- Squares Method** is based on the Bayes' theorem plus a maximum-likelihood condition.

$$\boxed{[\mathbf{y}\text{-}\mathbf{f}(\mathbf{p})]^{+}\mathrm{V}_{\mathrm{y}}^{-1}[\mathbf{y}\text{-}\mathbf{f}(\mathbf{p})]+[\mathbf{p}-\mathbf{p}_{\mathbf{0}}]^{+}\mathbf{V}_{\mathbf{0}}^{-1}[\mathbf{p}\text{-}\mathbf{p}_{\mathbf{0}}] = \mathrm{min}}$$

Note that prior and new information need to be independent!

Solution:

$$\mathbf{p}=\mathbf{p}_0+\mathbf{V}_0\,\mathbf{C}^{+}(\mathbf{Q}+\mathbf{V}_{\mathbf{y}})^{-1}[\mathbf{y}\text{-}\,\mathbf{f}(\mathbf{p}_0)],$$
$$\mathbf{Q}=\mathrm{C}\mathbf{V}_{\mathbf{0}}\mathrm{C}^{+},$$
$$\mathbf{V}_{\mathbf{p}}=\mathbf{V}_0\,\text{-}\,\mathbf{V}_{\mathbf{0}}\mathbf{C}^{+}(\mathbf{Q}+\mathbf{V}_{\mathbf{y}})^{-1}\mathbf{C}\mathbf{V}_{\mathbf{0}},$$
$$(\chi^2)_{\mathrm{min}}=[\mathbf{y}\text{-}\mathbf{f}(\mathbf{p}_{\mathbf{0}})]^{+}(\mathbf{Q}+\mathbf{V}_{\mathbf{y}})^{-1}[\mathbf{y}\text{-}\mathbf{f}(\mathbf{p}_{\mathbf{0}})].$$

Assuming that the model is ***linear***, i.e., $\mathbf{f}(\mathbf{p})=\mathbf{C}\mathbf{p}$.

An example: ^{239}Pu (n,f) and ^{235}U (n,f) cross sections below 20 MeV.

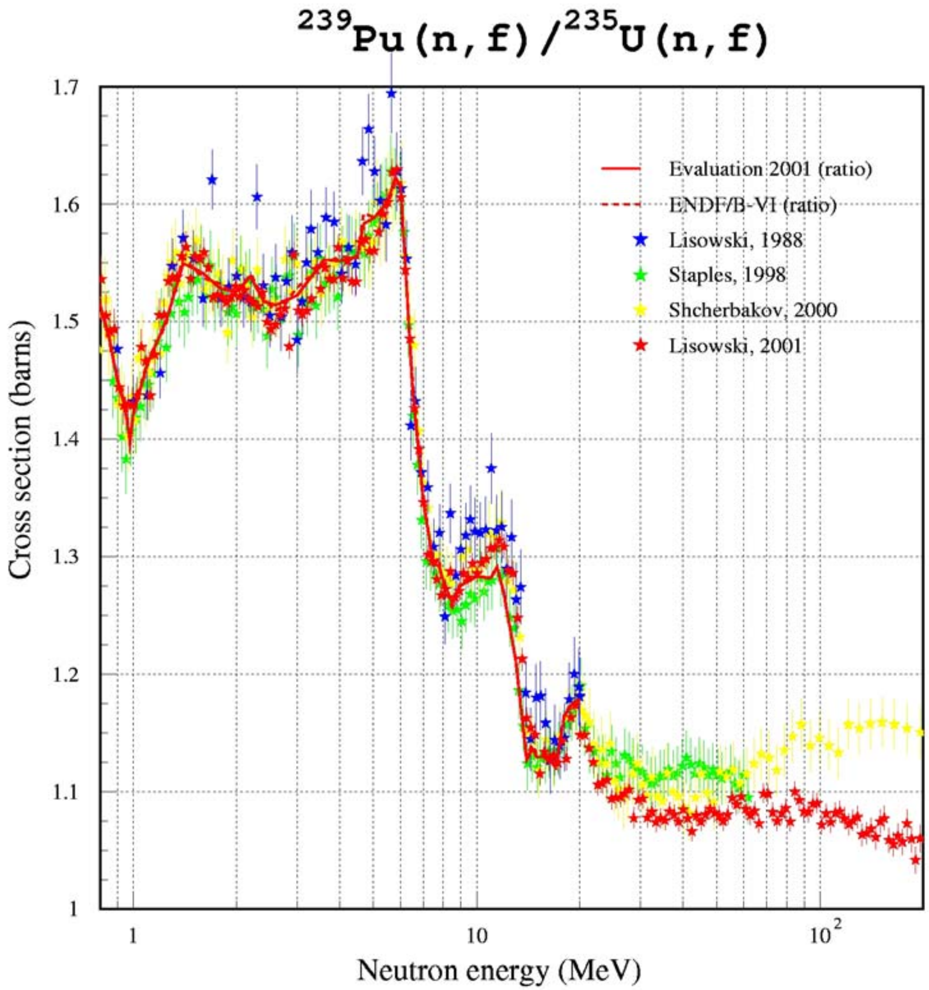
- ^{239}Pu is a very important isotope in the US nuclear stockpile;
  ^{235}U is a corner stone in almost every nuclear data evaluations (“ standard”).

- ^{239}Pu (n,f) experimental database used:
  - ~ 50 sets (~ 1000 energy points);
  - absolute and in ratio to ^{235}U (n,f);
  - includes very recent data sets (e.g., Lisowski 2001, LANSCE);
  - revisits older data sets.

- ^{235}U (n,f) experimental database:
  - Absolute measurements;
  - Shape measurements (no flux normalization for instance);
  - In ratio to light elements reactions.

One of the most difficult task of the evaluator is how to treat the experimental data correctly!

Some results

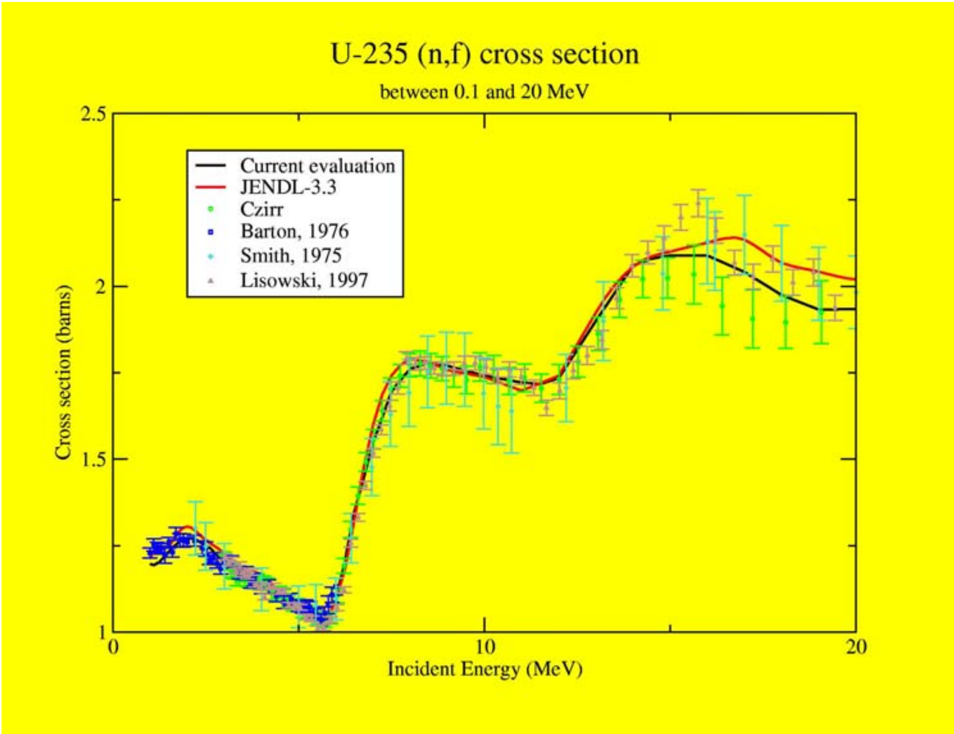


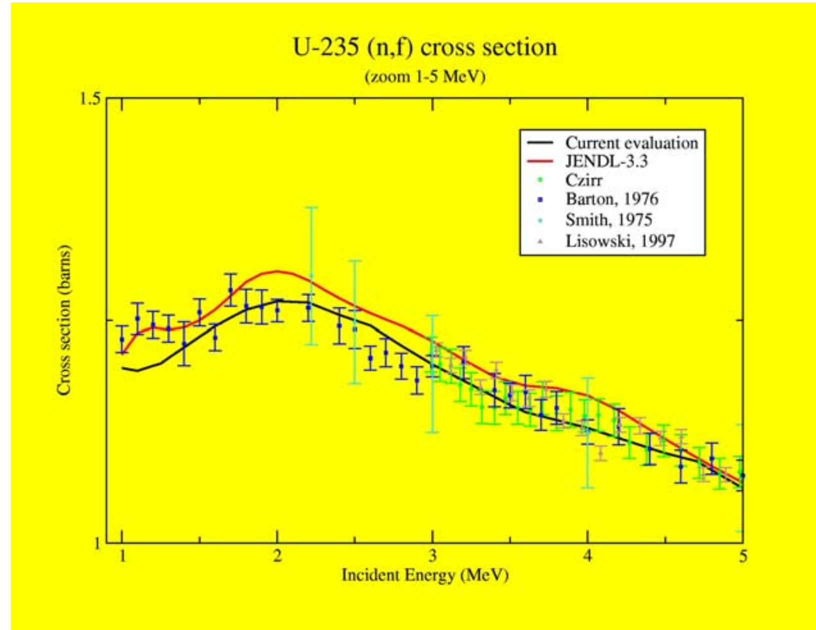
Fairly precise ratio evaluation below 20 MeV;

Resulting point- wise errors reduced from last evaluation (caution!);

Few (discrepant) experimental data sets beyond 20 MeV.

^{235}U (n,f) cross section





Point- wise uncertainties less than ~1% for both JENDL- 3.3 and the current evaluation;
BUT, these two evaluations differ by more than 3% in places!

The discrepancies come from *ad- hoc* correction of experimental data sets alone (the different mathematical tools give quite similar answers).

Improvements?

New tools:

Sensitivity analysis;
Robust inference (e.g., to deal with outliers);
Markov chain Monte-Carlo simulations.

What's next?

Future work:

New studies of neutron-induced fission cross sections of actinides present in the nuclear waste stream (e.g., ^{237}Np, ^{241}Am).

“I play at écarté with a gentleman whom I know to be perfectly honest. What is the chance that he turns up the king? It is 1/8. This is a problem of the **probability of effects**. I play with a gentleman whom I do not know. He has dealt ten times, and he has turned the king up six times. What is the chance that he is a sharper? This is a problem of the **probability of causes**. It may be said that it is **the essential problem of the experimental method**.”

- Henri Poincaré, “Science & Hypothe